Abstract Submitted
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Substitutional NaCl hydration in ice[1] PETER J. FEIBELMAN, Sandia National Laboratories — Na^+ and Cl^- can replace water molecules in ice Ih, with minimal lattice strain and without disrupting the crystal's H-bond network. *Ab initio* calculations show that substitutional solvation is optimally endothermic by only 0.50 eV per NaCl formula unit. Consistent with Na^+ and Cl^- ionic radii of 1.0 and 1.8 Å, Na^+ ions in the optimal structure lie 2.43 Å from their four equidistant, nearest O-atom neighbors, and the Cl^- ions 3.02 Å from theirs. Solvation of *interstitial* ions is less favorable by at least 1.5 eV. These results are cautionary for molecular dynamics simulations of ionic solvation in ice; a correction for the presence of water interstitials is needed if the number of molecules in the simulation cell is chosen too large, and another for the generation of free Bjerrum defects, if anion and cation solvation are treated separately.

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Peter J. Feibelman
Sandia National Laboratories

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